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SIMPLIFIED GROUNDWATER FLOW MODELING: AN APPLICATION OF KALMAN FILTER BASED IDENTIFICATION*

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The need exists for methods to simplify groundwater contaminant transport models. Reduced-order models are needed in risk assessments for licensing and regulating long-term nuclear waste repositories. Such models will be used in Monte Carlo simulations to generate probabilities of nuclear waste migration in aquifers at candidate repository sites in the United States.

In this feasibility study we focused on groundwater flow rather than contaminant transport because the flow problem is more simple. A pump-drawdown test is modeled with a reduced-order set of ordinary differential equations obtained by differencing the partial differential equation. We determined the accuracy of the reduced model by comparing it with the analytic solution for the drawdown test. We established an accuracy requirement of 2% error at the single observation well and found that a model with only 21 states satisfied that criterion. That model was used in an extended Kalman filter with synthesized measurement data from one observation well to identify transmissivity within 1% error and storage coefficient within 10% error. We used several statistical tests to assess the performance of the estimator/identifier and found it to be satisfactory for this application. This feasibility study highlighted problems known to others who have attempted to apply modern systems methods to hydrological problems and has led to related research studies at our laboratory.

INTRODUCTION

Lawrence Livermore Laboratory has worked for some time on research for the U.S. Nuclear Regulatory Commission (NRC). One of the studies for the NRC has been the Waste Management Program. That program supplies technical support to the NRC for making licensing and regulatory decisions for candidate nuclear waste repository sites under consideration in the United States. Central to that work are studies in assessing risks of alternate decisions. The program has developed a sophisticated network of models that include all steps in the nuclear waste isolation process and that eventually provide estimates of dose to man.

On the request of the Waste Management Program, a group in the engineering departments at Livermore carried out the pilot project that is summarized in this paper in an attempt to lay out a more formal research program in this area in the future. The scope of this pilot project was intentionally chosen to be narrow so that fruitful results could be demonstrated. We began by postulating a pump-drawdown problem where we felt we could mechanize the process of identifying aquifer parameters from drawdown data through the use of signal-processing techniques. After getting ideas from the literature and from others in the field, we initiated the study described in what follows. We wanted to demonstrate the power of modern statistical techniques applied to problems in groundwater flow and transport. One of the things we eventually wanted to show was a comparison between what our methods could do and what is routinely done by geoscientists in the field. For that reason we chose a problem for which the true answer was known beforehand and one that was familiar to practicing hydrologists.

We modeled what would happen if a Kalman filter based estimator/identifier were used with on-line measurements from a single observation well to identify aquifer parameters from noisy measurement data. The whole process involved defining and narrowing the scope of the problem, finding a large-scale numerical or analytical model to use as a "truth" model for accuracy comparisons, adopting a method of transforming partial differential equations for groundwater flow into sets of ordinary differential state equations, implementing estimator/identifiers that used those state equations to determine the system parameters, assessing the applicability of the methods used, and suggesting areas for future research.

The topic of this paper is germane to the IFIP Working Conference. It is an example of a study that brought together engineers, scientists, and numerical mathematicians to work on a problem of common interest in the environment, much as does the working conference itself. We only regret that at the last minute we found we were unable to present this paper in person, and that it took so long in its final preparation.

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HYDROGEOLOGICAL MODEL DEVELOPMENT

In this section we discuss the development of a hydrogeological model used to determine properties of a simulated aquifer. This model will be employed in an estimation scheme to identify transmissivity and storage coefficients.

The pump-drawdown test is a fundamental technique used in aquifer tests to determine hydrogeological properties. The effect of pumping water from a well at a known rate is measured in distant observation wells penetrating the aquifer (see Figure 1). The purpose of the test is to determine relationships among pumping rate, drawdown (lowering of the water table), and time in order to estimate the desired physical properties from these data.

Consider developing a mathematical representation of the pumping test depicted in Figure 1. We assume that the aquifer is: (1) confined; (2) of infinite areal extent; (3) homogeneous; (4) isotropic; and (5) of uniform thickness. Also, we assume that the wells completely penetrate the aquifer, are of negligible diameter, and flow is radial. The pump rate is assumed constant.

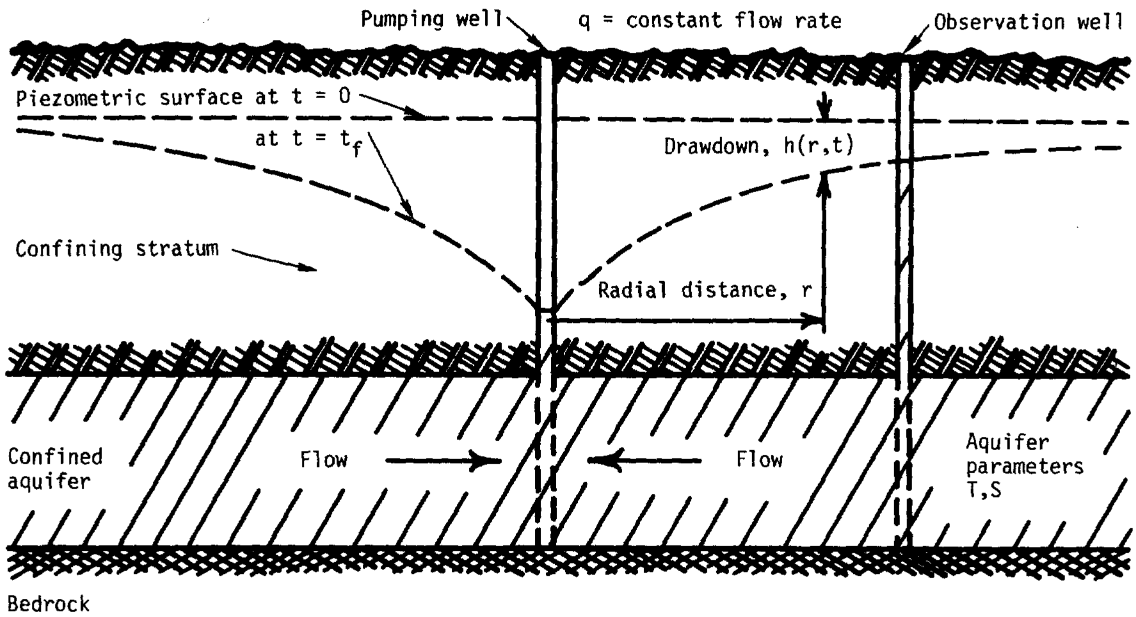

Figure 1. In an aquifer pump-drawdown test (Theis (1935), Jacob (1950), DeWiest (1966), Davis and DeWiest (1966)), the effects of pumping water on the piezometric surface are measured at an observation well in order to infer the aquifer transmissivity (T) and storage coefficient (S).

When the pumping well in the aquifer is operated, water is continuously withdrawn from storage within the aquifer as the cone of depression in the piezometric surface progresses radially outward from the well. This water is released by the compaction of the aquifer and its associated beds, and by the expansion of the water itself. Assume that the water is released instantaneously with a decline in head caused by decreasing pore pressure. Then the groundwater flow in polar coordinates is given by (Davis and DeWiest (1966)):

$$\frac{\partial h(r,t)}{\partial t} = \left(\frac{T}{rS}\right)\frac{\partial}{\partial r}\left[r\,\frac{\partial h(r,t)}{\partial r}\right] \quad \text{(m/s)}, \tag{1}$$

where

$h(\cdot)$ = drawdown (m),
r = radial distance from the pumping well (m),
T = transmissivity (m^3/Pa-s),
S = coefficient of storage (m/Pa),
t = time (s).

The initial condition for $r \geq 0$ is given by

$$h(r,0) = h_0 = 0 \text{ (m)}.$$

Boundary conditions for $t \geq 0$ are defined by

$$\lim_{r\to\infty} h(r,t) = h_0 = 0 \text{ (m)},$$

$$\lim_{r\to 0} \left[r \frac{\partial h(r,t)}{\partial r} \right] = \frac{q}{2\pi T} \text{ (m)},$$

where q = constant (m^3/s) is the pumping rate. The groundwater flow equation can be converted to a finite set of differential-difference equations by approximating with finite differences. Using central differences, we obtain the following general differential-difference equation:

$$\dot{h}_i = \frac{T}{r_i S} \left(\frac{1}{r_{i+1} - r_{i-1}} \right) \left[(r_{i+1} + r_i) \left(\frac{h_{i+1} - h_i}{r_{i+1} - r_i} \right) - (r_i + r_{i-1}) \left(\frac{h_i - h_{i-1}}{r_i - r_{i-1}} \right) \right], \tag{2}$$

where each of the states h_i in (2) is a function of distance and time, $h_i \equiv h(r_i,t)$. This expression may be rewritten as

$$\dot{h}_i = T/S \left[C_{i3}h_{i+1} - C_{i2}h_i + C_{i1}h_{i-1} \right], \text{ for } 1 < i < N, \tag{3}$$

where

$$C_{i3} = \frac{r_i + r_{i+1}}{r_i(r_{i+1} - r_i)(r_{i+1} - r_{i-1})},$$

$$C_{i2} = \frac{2}{(r_{i+1} - r_i)(r_i - r_{i-1})},$$

$$C_{i1} = \frac{r_{i-1} + r_i}{r_i(r_{i+1} - r_{i-1})(r_i - r_{i-1})}.$$

The boundary conditions are included in the following way. As $r\to 0$, the pump is included as part of a step input of magnitude $q/2\pi T$(m). As $r\to\infty$, the pressure is essentially constant at the boundary; therefore, the last node N is chosen to lie at a distance from the pumping well that is much greater than that of the observation well.

Thus we have

$$\dot{h}_N = -\left(\frac{T}{S}\right) C_{N2}h_N + \left(\frac{T}{S}\right) C_{N1}h_{N-1}{}^{*}.$$

The state representation of the groundwater flow equation is given by

$$\dot{h}_i = \begin{cases} (T/S)C_{13}h_2 - (T/S)C_{12}h_1 - (\frac{1}{S})C_{11}q\,\mu(t), & i = 1; \\ (T/S)C_{i3}h_{i+1} - (T/S)C_{i2}h_i + (T/S)C_{i1}h_{i-1}, & 1<i<N; \\ -(T/S)C_{N2}h_N + (T/S)C_{N1}h_{N-1}, & i = N. \end{cases} \tag{4}$$

The coefficients are given by:

$$C_{13} = \frac{1}{r_1(r_2 - r_1)},$$

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*Actually the boundary condition $\lim_{r\to\infty} h(r,t) = 0$ is equivalent to the condition $\lim_{r\to\infty} \left[r \frac{\partial h(r,t)}{\partial r} \right] = 0$, which is incorporated into the equation for h_N (see Azevedo et al. (1980) for details).

$$c_{12} = c_{13} ,$$

$$c_{11} = \frac{1}{\pi r_1(r_2 + r_1)} ,$$

$$c_{N2} = \frac{r_N + r_{N-1}}{\lambda r_N(r_N - r_{N-1})^2}, \ \lambda \text{ a constant}^{\dagger} ,$$

$$c_{N1} = c_{N2} ,$$

c_{ij}, j = 1,2,3, are defined in (3) ,

$\mu(t)$ = unit step function in time.

These equations form a set of first-order ordinary differential equations of the general continuous state space form:

$$\dot{x}_t = F_t x_t + G_t u_t .$$

Discrete measurements are given by: (5)

$$y_k = H_k x_k .$$

In (5), x, u, and y are the n-state, m-input, and p-output vectors and F, G, and H are matrices of appropriate dimension.

Finally, for this general state-space form in (5), the groundwater flow equation becomes:

$$\dot{x}(r,t) = F(r)x(r,t) + g(r)u(r,t), \tag{6}$$

where

$$x^T(r,t) = \left[h(r_1,t),\ldots,h(r_N,t)\right],$$

$$u(r,t) = \mu(t),$$

$$F(r) = \left(\frac{T}{S}\right) \begin{bmatrix} -c_{12} & c_{13} & & & & & 0 \\ c_{21} & -c_{22} & c_{23} & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & c_{i1} & -c_{i2} & c_{i3} & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & c_{(N-1)1} & -c_{(N-1)2} & c_{(N-1)3} \\ 0 & & & & & c_{N1} & -c_{N2} \end{bmatrix} ,$$

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†The constant λ is used to adjust $h(r_N,t)$ incorporating the boundary effects using non-uniform node spacing for $r >> r_N$ (see Azevedo et al. (1980) for details).

$$g(r) = \begin{bmatrix} -C_{11}q/S \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Notice that the structure of the F matrix and g vector in (6) hint at the fact that the responses for this system will be very well-behaved. The F matrix is banded with all diagonal terms negative. Thus, its poles will all be negative real and the entire system will be absolutely stable in its time response. The spatial discretization has led to a system of coupled, first-order lags, so that system response will be very simple and non-oscillatory.

The measurement equation representing the observation well at node r_w (w is well node number) is

$$y_k = H_k x_k, \tag{7}$$

where $H_k = e_w^T$, a unit row vector. Construction of the standard observability matrix (Takahashi et al. (1970)) shows that the system is completely observable from the observation well; i.e., from the drawdown measurements at the well $\{y_k\}$, it is possible to reconstruct the drawdown of all of the states $\{h(r_i,t)\}$.

Before we discuss the state simulation of this groundwater flow equation, consider the closed form solution of (1). It can be shown (Theis (1935)) that:

$$h_{TRUE}(r,t) \equiv h(r,t) = h_o - \frac{q}{4\pi T} \int_{\frac{r^2 S}{4Tt}}^{\infty} \frac{e^{-\delta}}{\delta}\, d\delta \,. \tag{8}$$

We define the solution expressed in this equation as our "truth" model and use it to compare with the solution of the state differential-difference equations. A typical simulation of the groundwater flow model is shown in Figure 2 for the nodes at the pumped and observation wells and at a distant node that is near the boundary. The parameters for the model used in the simulation are given in Table 1.

Table 1. Simulation Parameters*

Transmissivity (m^3/Pa-s)	1×10^{-8}
Storage Coefficient (m/Pa)	5×10^{-7}
Pump Rate (m^3/s)	1×10^{-2}
Radial Distance (m)	
Observation Well	1×10^{2}
Boundary	5×10^{4}

*These values were suggested for this pilot study by L. D. Thorson, a hydrological systems modeler at LLL.

Simulated drawdown from the spatially-discretized model yields relative modeling errors† of less than 2% at node 10, the observation well, indicating a close agreement between the analytical or "true" solution and that from the model.

The reader should note that a modeling tradeoff exists: increased accuracy in the finite-difference solution results only from inclusion of an increased number of nodes in the model. We decided on using 28 nodes or states in our model based on simulation experiments and it is that level of model sophistication that resulted in the errors mentioned above.

Essentially we are truncating a spatially infinite system to obtain a finite approximation for computer processing. In the infinite system, $\lim_{r\to\infty} h(r,t) = 0$ for all t, but for the finite approximation, we must constrain $h(r_{N+1}, t) \equiv 0$ where $r_{N+1} < \infty$. If this boundary node is situated too close to the observation well, reflections will occur due to poor boundary modeling.

†The relative error is defined by $\epsilon_{REL} \equiv \dfrac{h_{TRUE} - h_{MODEL}}{h_{TRUE}}$.

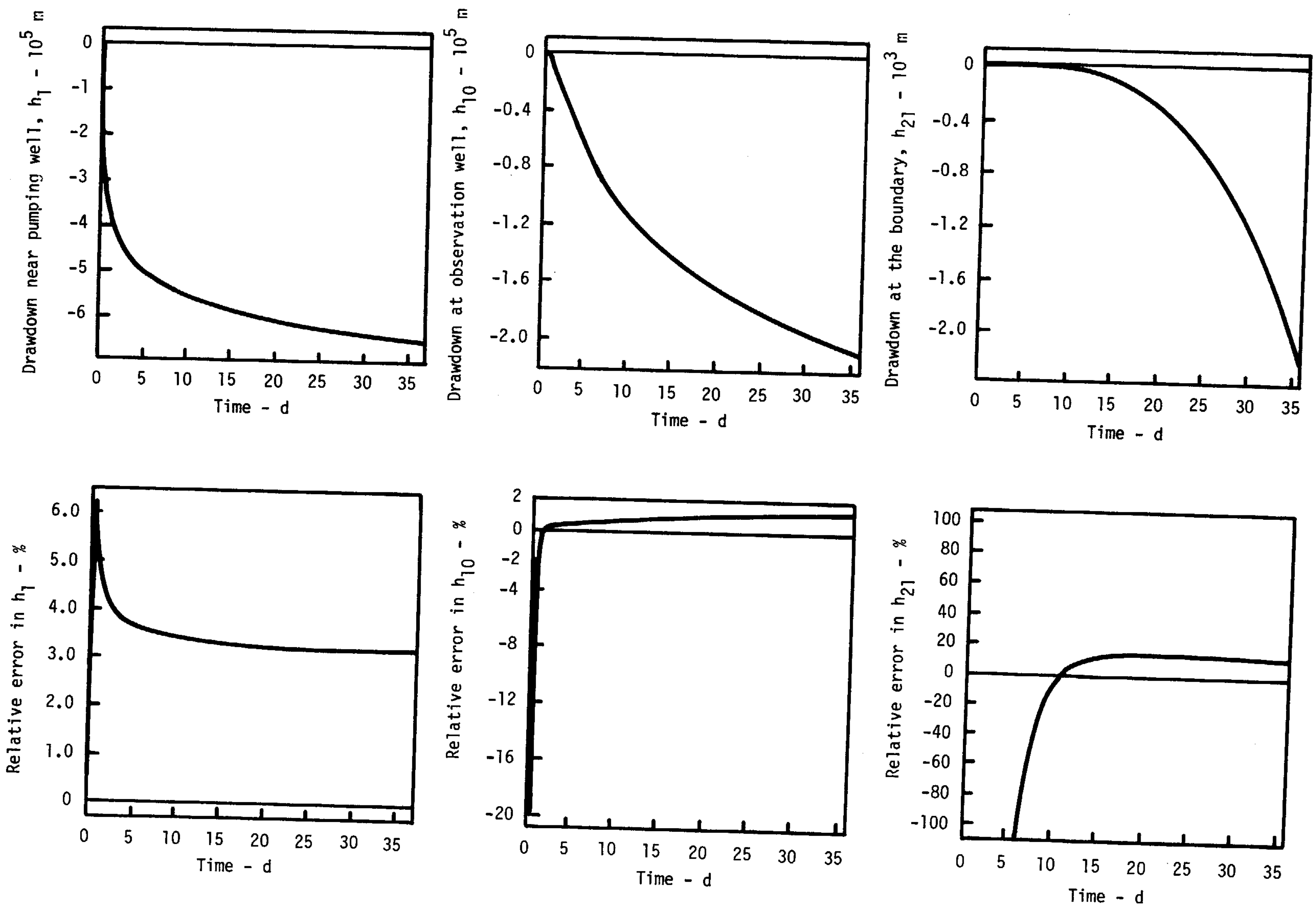

FIGURE 2. Simulated drawdown near the pumping well, at the observation well, and at the boundary node showed adequately small modeling errors relative to the analytical solution for a model with only 28 states.

Thus, the 28-state model was chosen such that the analytically-derived drawdown at the hypothetical 28^{th} state is considerably smaller (~ 2 orders of magnitude) than that at the observation well node. Then, setting node 28 to zero in the spatially discretized model does not significantly alter the observation well drawdown.

Figure 3(a) shows the spatial distribution of the drawdown using the discretized model at six different times. This is a good illustration of the "cone of depression" dynamics for the simulated aquifer. Notice that the boundary node has very small drawdown values compared to the nodes very near the pump and at the observation well. Figure 3(b) is a plot of the relative error between analytic and finite-difference models at the final time ($t_f \cong 35$ d). Again, reasonable agreement (less than 2% error) between models is observed in the region of the observation well. Details of the modeling and simulations are discussed in Azevedo et al. (1980).

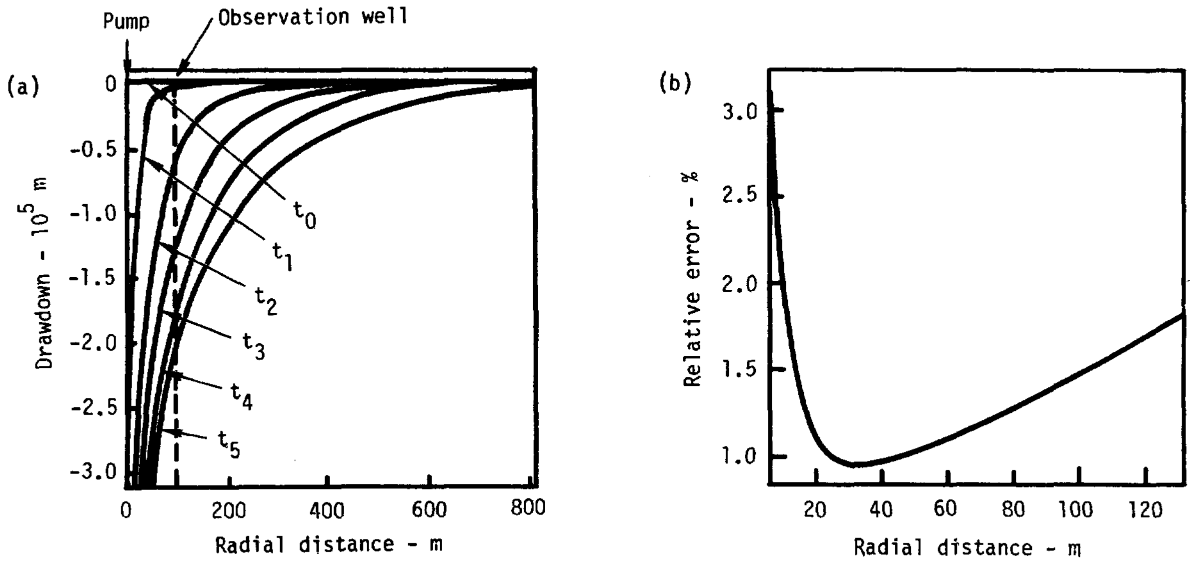

Figure 3. The cone of depression is shown forming for several times in (a). The relative error between the true and simulated solutions is shown in (b) at the final time (35 d) of the run shown in Figure 2.

ESTIMATOR/IDENTIFIER DESIGN

In this section we consider the design of an on-line state and parameter estimator/identifier. We choose to "reconstruct" the drawdown at various spatial points as well as estimate the aquifer's physical parameters. The drawdown estimates could eventually be used as sample points for groundwater level contour mapping (Olea (1974)). The general state estimation/parameter identification problem is:

Given: a set of noisy measurements $\{z_k\}$ from a nonlinear dynamical system

$$\dot{h} = f(h, \theta) + g(u, \theta) + w_\theta$$

and discrete-time measurement system

$$z_k = h(h, \theta) + v_\theta , \qquad (9)$$

where h, u, z, θ are the n-state, m-input, p-output, and q-parameter vectors with associated nonlinear functions f(•), g(•), h(•), and $w_\theta \sim N(0, Q_\theta)$*, $v_\theta \sim N(0, R_\theta)$.

Find: the "best" (minimum variance) estimates $\hat{h}, \hat{\theta}$ of h and θ (Gelb (1974)).

Before we discuss the solution to this problem, consider the model of the drawdown measurement system. We assume that a steel tape is used to measure the drawdown (Davis and DeWiest (1966)). The measurement model is given by

*This notation, $\bar{x} \sim \bar{N}(x, \epsilon_x)$, means x is distributed normal with mean $\bar{x}$ and covariance ϵ_x.

$$z_k = y_k + v_k \; , \tag{10}$$

where $v_k \sim N(0, R_k)$ and y_k is defined in (7). A 10% of full scale ($\sim 10^5$ m) random error was simulated as a severe test to investigate how well the estimator/identifier could perform. Simulated measurement data is shown in Figure 4.

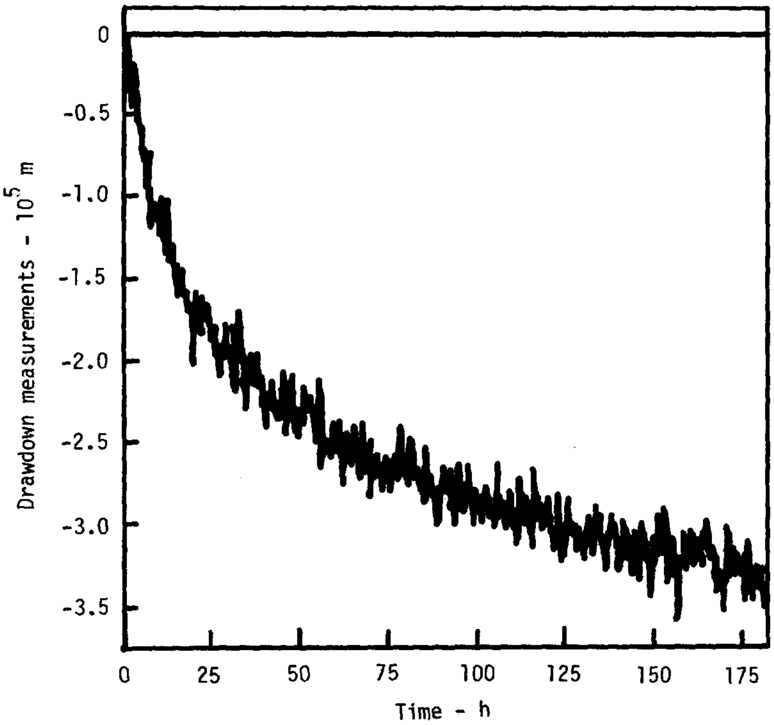

Figure 4. This is simulated noisy measurement data of drawdown at the observation well, 100 m from the pumping well, when the level of measurement error is set at 10% of full scale in the 28-state model ($R = 10^8$ m^2).

In order to solve the on-line state estimation/parameter identification problem of (9), an extended Kalman filter (EKF) was constructed (Gelb (1974), Jazwinski (1970)); see Castleton and Candy (1979) for details of our EKF.

The estimator/identifier was implemented with the necessary Jacobians using data generated by the 28 node model. The model used in the estimator consisted of 21 nodes (states). Initially, the transmissivity and storage coefficient were "guessed" with large errors (> 100%), and the states and parameters were estimated well (< 10% relative error). However, in order to conserve computational time for this feasibility study, the initial errors were selected from a Gaussian distribution with true mean and 25% error variance, i.e., $\tilde{x}_0 \sim N[x_{TRUE}, (0.25x_{TRUE})^2]$. An ensemble of ten runs was generated; a typical member simulation is depicted in Figures 5 and 6. In Figure 5, we see the "reconstructed" drawdown estimates with associated estimation error curves ($\tilde{x} := x_{TRUE} - \hat{x}$) and 2-sigma bounds predicted by the estimator (i.e., the 95% confidence limits). We see that initially the drawdown estimates are in large error due to the uncertainty in the parameters, but eventually they track. In fact, in steady state the variances are $\tilde{\pi}_1^{1/2} \approx 2 \times 10^3$m and $\tilde{\pi}_{10}^{1/2} \approx 7 \times 10^2$m, which are quite reasonable. Simultaneous parameter estimates of transmissivity and reciprocal storage coefficient ($S_R = 1/S$) are also shown for this run in Figure 6. Here we see the estimates with associated estimation errors. For this run the estimator performed quite well with relative errors of approximately 0.3% and 8.5% respectively for T and S_R. The ensemble results are shown in Table 3 and the constant probability contour (Azevedo and Gavel (1980)) of the estimates are shown in Figure 7. Note that the ellipse has collapsed visually to a line centered at the sample mean due to scaling. The 3-σ ellipse contains the sample estimates ($\hat{T}$, $\hat{S}_R$) with a probability of 0.99.

RESULTS

This pilot study has shown several things, both good and bad. Our initial naivete in the area of groundwater systems is very apparent from some of the numerical simulations shown in the figures. The standard set of model parameters given us by a colleague at LLL who is experienced in the application

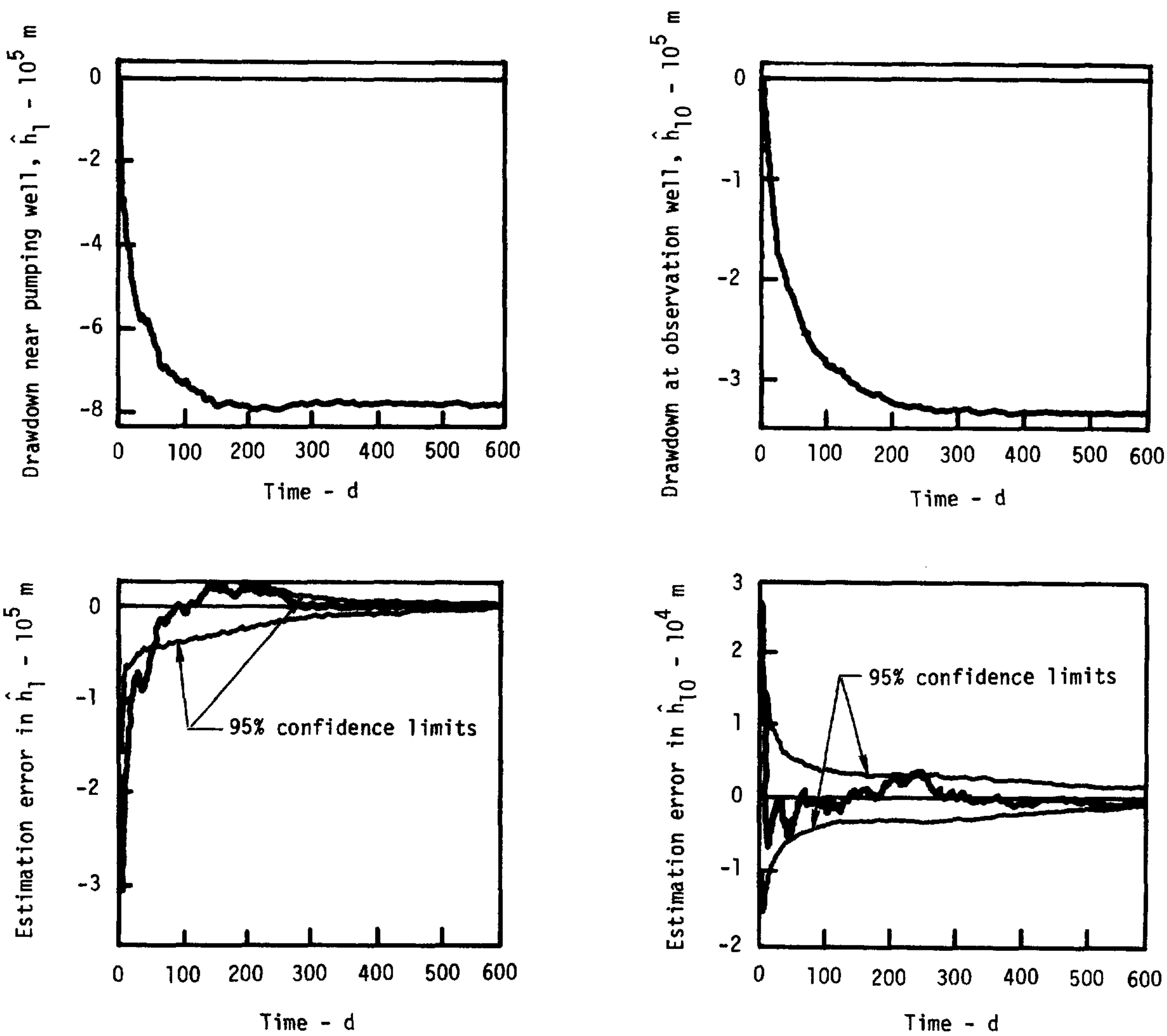

Figure 5. Drawdown estimates near the pumping well (h_1) and at the observation well (h_{10}) were generated with the extended Kalman filter using a 21-state model in the filter. Estimation errors show that the filter is performing well when using synthesized measurement data from a 28-state model.

Table 3. Identified parameter sample statistics for an ensemble of 10 runs.

PARAMETER	TRUE VALUE (x_{TRUE})	ESTIMATED MEAN ($\bar{x}$)	STANDARD DEVIATION ($\sigma_{\hat{x}}$)	MEAN ERROR (BIAS) ($\tilde{x}$)	% MEAN ERROR ($\tilde{x}$, %)	ERROR STD ($\sigma_{\tilde{x}}$)	MAX ERROR (x_{max})	MIN ERROR (x_{min})
T ($\times 10^{-8}$)	1.00000	1.00510	.00070	-.00510	.510	.00070	.00579	.00376
$S_R(=1/S)$ ($\times 10^{6}$)	2.00000	2.07380	.00319	-.07380	7.380	.00319	.07662	.06754

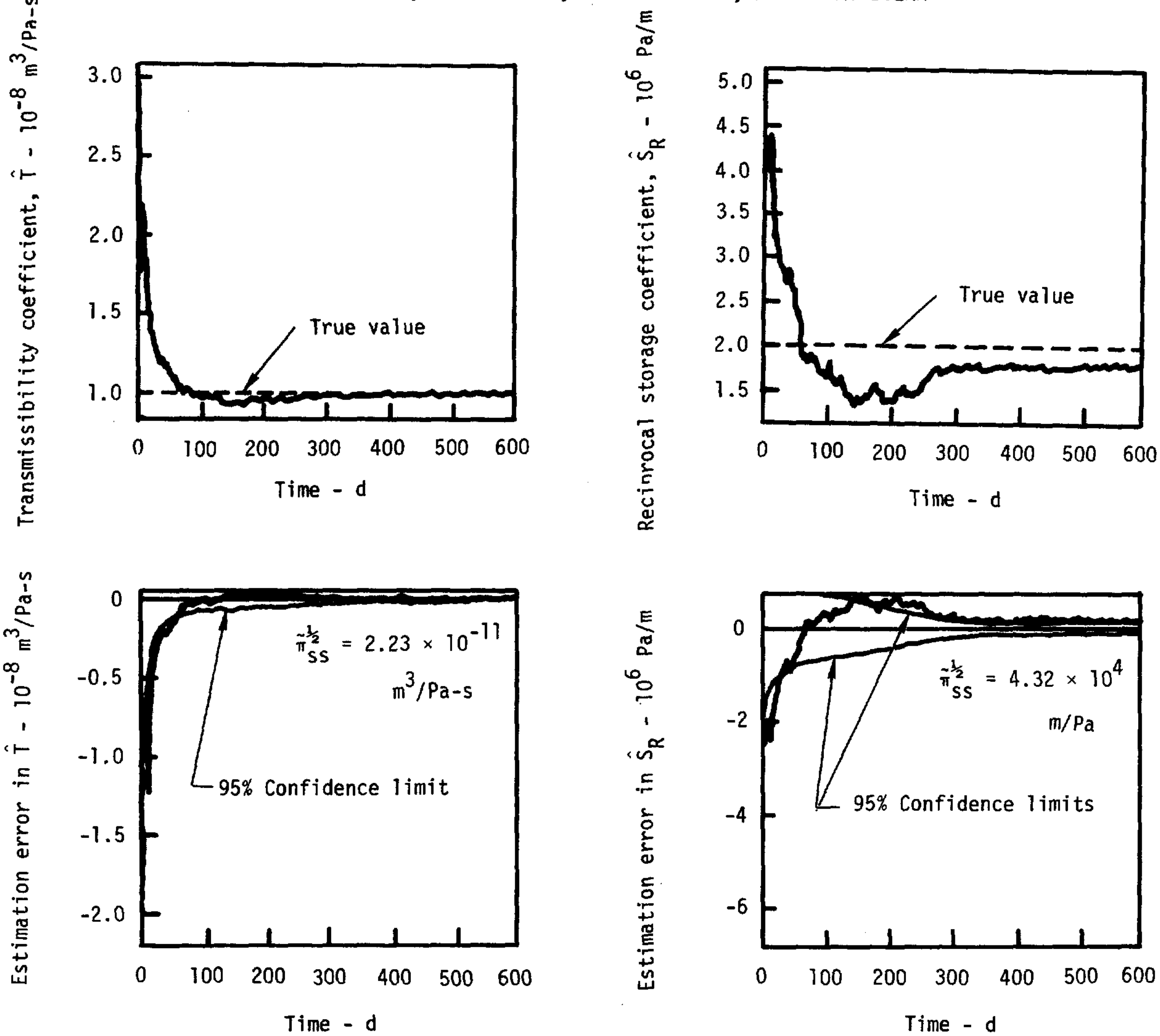

Figure 6. Results of the parameter identification for transmissivity (T) and reciprocal storage coefficient (S_R = 1/S) indicate the extended Kalman filter is tracking T within 1% error and S within 10% error.

of flow models in tight, impervious aquifer systems led to horrendously large drawdown values. Once we tuned the simulations to yield interesting time histories that looked like they would prove useful for parameter identification, we picked a significant measurement error merely for testing purposes that would correspond to 10% of the full-scale drawdown. But 10% of the kinds of excursions we were getting yielded an error of 10^5 m! That is an uncertainty of more than 50 miles for a steel tape measurement! Clearly this is absurd, but for demonstration purposes, the concepts still all work out. In hindsight, if we in fact have a system with parameters defined to be in the ranges of those in Table 1, then for a constant pumping rate of 1 x 10^{-2} m^3/s, pumping on an aquifer with a miniscule storage coefficient of 5 x 10^{-7} m/Pa quite naturally leads to tremendously large drawdown values. Because in order to get 10 l/s out of rock that can store only 0.5 ml/Pa, you have got to reduce the piezometric head by tens of thousands of meters.

This initial oversight in parameter values does point up a real problem that has been seriously bothering those who are actively working in the nuclear waste repository licensing area. And that is: how do you even begin to make credible geophysical measurements to determine aquifer-type constants when the media in which repositories are being designed are by definition *non*-aquifers? Classical drawdown and packer tests may prove to be completely useless with systems whose parameters are in the ranges of those in this study. Notice also that the results indicated in Figures 5 through 7 took months of simulated time due to the tightness of the modeled aquifers; this would be clearly prohibitive in actual field tests.

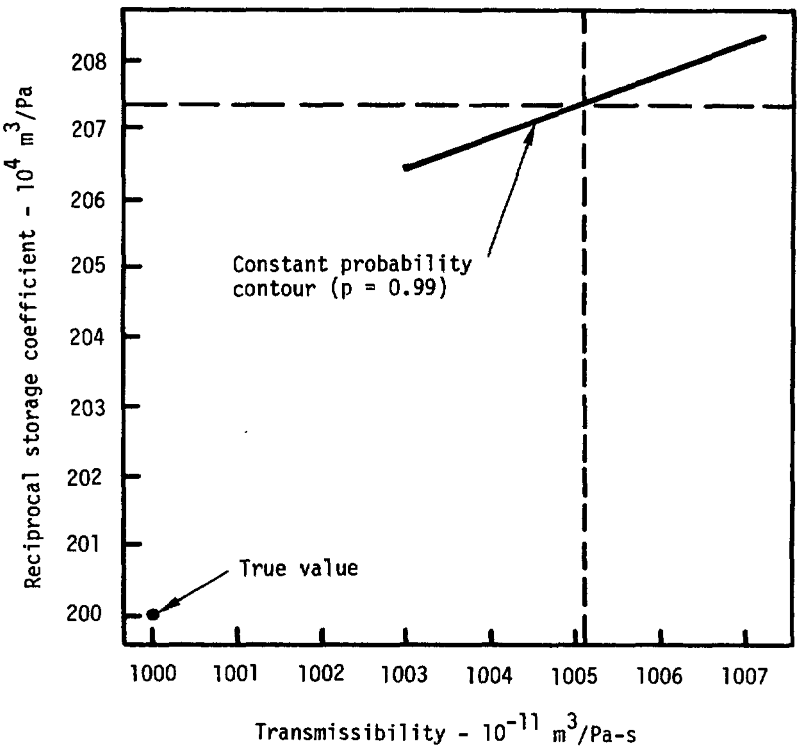

Figure 7. The accuracy and precision of the parameter estimates generated from the ensemble runs are shown in this figure.

It seems as though we have uncovered a problem area in approaching this simple test from the stochastic systems point of view that the classical hydrogeologists have known well for some time. With the current interest in exotic geologies for siting waste repositories, new geophysical measurement methods may have to be developed to acquire data because the techniques that were spawned in studies of free-flowing aquifers were really for entirely different physical regimes and may not apply. This points up an area where the stochastic systems scientist might well come to the aid of the hydrologist in future research for repository licensing.

The only other major shortcoming of the approach taken here was in the dimensionality of the model used in the system. Distributed-parameter systems always involve large models in order to achieve rich detail in simulation results. Our problem was perhaps the simplest case and it took a model with over 20 states to function properly. Once we go to two and three spatial dimensions and variable parameters, the model dimensionality problems will soon swamp the capabilities of what can be feasibly done with the extended Kalman filter approach. This result aligns with that of McLaughlin (McLaughlin (1978)).

What this study does show is that parameters can be reasonably identified with this approach provided the models required do not get too complex. The result is encouraging and stimulates us to look into allied statistical methods for more realistic applications. Some of these methods we are now considering include maximum likelihood identification and kriging techniques.

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